

# Improved Accuracy and Uncertainty Management for High-Speed and Unsteady Flows using Optimization Techniques

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## Executive Summary

The goal of this project was to demonstrate the potential of adjoint methods for improving the accuracy of current simulation capabilities and to enable more effective uncertainty quantification techniques. A major portion of this project was targeted towards developing modular adjoint formulations which can be extended to relatively complex simulation problems such as real gas hypersonic simulations, unsteady problems, and unsteady multidisciplinary problems such as aeroelasticity. The modular adjoint approach developed in this work has been applied to the following problems: optimized mesh deformation techniques, hypersonic discretization error reduction through h-p adaptive techniques, real-gas hypersonic simulations, unsteady transonic flow simulations, and unsteady fully coupled aeroelastic problems. In addition to formulating and solving the adjoint problem for all these cases, this work has demonstrated the potential of adjoint-produced sensitivities for efficiently solving time-dependent optimization problems, including fully coupled aeroelastic problems, as well as the potential for adjoint methods for providing error estimates which can be used to drive adaptive meshing or time stepping procedures and/or for performing uncertainty quantification. This project resulted in two PhD theses, the first one (partially supported) based on the demonstration of control of discretization error for hypersonic flow using adjoint techniques, and the second PhD thesis based on the demonstration of unsteady optimization problems as well as the demonstration of adjoint-driven adaptive time step and convergence tolerance criteria for controlling errors in time-dependent problems.

## 1. Introduction

Computational methods have been playing an increasingly important role in aerospace vehicle analysis and design over the last several decades, due to the rapidly advancing capabilities of computer hardware, as well as increasingly sophisticated and capable numerical algorithms. For cases such as unsteady and/or high-speed flows, where properly scaled experimental simulation may be either expensive or unfeasible, numerical simulations can be particularly enabling.

However, in spite of the rapid advances and acceptance of numerical simulations, serious deficiencies remain in terms of accuracy, uncertainty, and validation for many applications. For hypersonic flows, surface heating is known to be particularly difficult to capture accurately, especially using unstructured grids, which are often favored for their ease of dealing with complex geometries. For unsteady flows, multiple error sources contribute to solution uncertainty, including spatial discretization errors, temporal discretization errors, and algebraic errors due to the usual practice of only partially converging the implicit system at each time step for time-implicit methods.

Sensitivity analysis techniques can be used to quantify errors in high speed and unsteady flow problems and to drive adaptive techniques with the goal of efficiently reducing the errors and thus uncertainty in these simulations. Sensitivity analysis based on adjoint methods have become popular in CFD simulations over the last decade. These methods were initially adopted for use in design optimization problems and more recently have been used for error estimation and adaptive mesh refinement purposes. Adjoint methods enable the calculation of the sensitivities for a single simulation output with respect to any number of simulation inputs at the cost of a single solution of the adjoint equations. Adjoint formulations can be obtained by transposing the linearization process, and are thus often thought of as reverse linearization techniques. For error estimation purposes, adjoint methods provide a mechanism for determining the effect of local errors (in space and time) on the final global simulation output of interest, as well as the sensitivity with respect to model parameters, such as empirically determined reaction rates in real gas models.

The goal of this work was to demonstrate the utility of adjoint-based techniques for computing sensitivities and estimating errors in important engineering quantities such as force coefficients and surface heating for high-speed flows, in the context of more complex unsteady and multi-disciplinary simulations.

## 2. Objectives

The objectives of this project were based on providing improved prediction capabilities and design optimization techniques for difficult problems of current concern to the USAF, including aerodynamic heating predictions for hypersonic vehicles and unsteady aeroelastic effects. This has been accomplished using adjoint-based techniques for estimating the error and calculating the sensitivities of the important engineering outputs for these problems. A secondary objective of this work was the demonstration of modular approaches for formulating, solving, and deploying adjoint methods for complex multi-disciplinary simulations involving real gas physical models and unsteady problems with deforming boundaries such as aeroelastics. The goals of this work are:

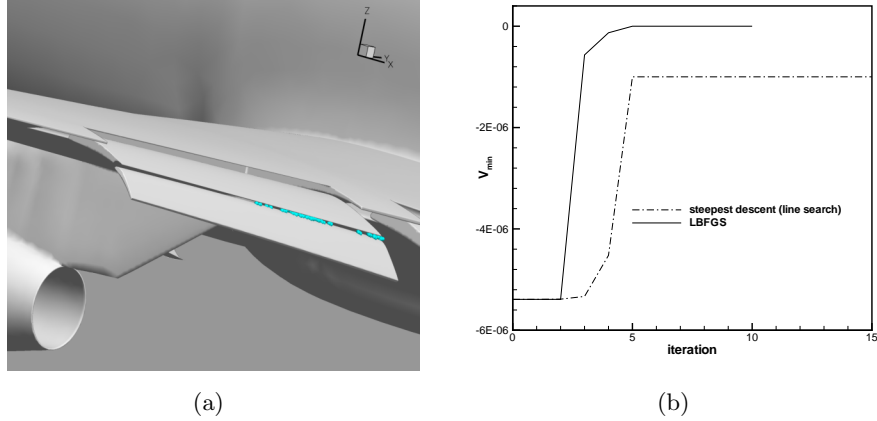
- Improved robust mesh deformation techniques for unsteady aeroelastic problems
- Improved heating predictions for perfect and real gas models, and design optimization strategies for such problems.

- Temporal error control strategies and design optimization strategies for unsteady problems with moving meshes and aeroelastic problems.

### 3. Accomplishments

#### 3.1 Mesh Motion

Dynamically deforming meshes are required for time-dependent problems with relative body motion, such as aeroelasticity or store separation problems, as well as for shape optimization problems where an ability to smoothly deform the geometry is required. Robust mesh deformation strategies are required in order to produce deformed valid meshes with no negative volume cells. The linear elasticity approach for mesh deformation has been shown to result in a relatively robust method, since in regions of very stiff cells (i.e. high modulus of elasticity  $E$ ) this approach produces solid body translation and rotation, and thus avoids element deformation. However, the success of the method is critically dependent on an appropriate distribution of the modulus of elasticity  $E$  on the mesh, with small cells near the body requiring large  $E$  values in order to avoid excessive deformation. While most approaches assume a suitable distribution of  $E$ , such as  $E$  being inversely



**Figure 1:** (a) Location of negative cells produced by mesh deformation solution using prescribed modulus  $E$  distribution on full aircraft configuration undergoing flap motion; (b) Convergence of the various optimization strategies as measured by the number of optimization cycles requires to recover mesh with fully positive volume cells.

proportional to the cell volume, the approach proposed in this project consists of developing an “optimal” distribution of  $E$  through design optimization techniques. An optimization problem is formulated where a scalar objective which provides a measure of overall grid quality is constructed, and the sensitivity of this objective with respect to the  $E$  value in each mesh cell is constructed using the discrete adjoint. The distribution of  $E$  is then optimized in such a way that the objective value is minimized, resulting in an  $E$  distribution which produces more robust and valid deformed grid configurations. Figure 1(a) illustrates a mesh deformation problem about a complete aircraft configuration reproduced from references [5,14]. This complex geometry was chosen as representative of a difficult mesh deformation problem. The wing and flaps are given a prescribed twisting motion which results in the negative cells shown in the gap regions, using a linear elasticity approach with a modulus  $E$  prescribed as inversely proportional to the cell size. Figure 1(b) illustrates

the optimization procedure, where the negative volume cells are seen to be eliminated after of the order of five design optimization cycles, using either a line-search approach, or the more powerful LBFGS optimization method.

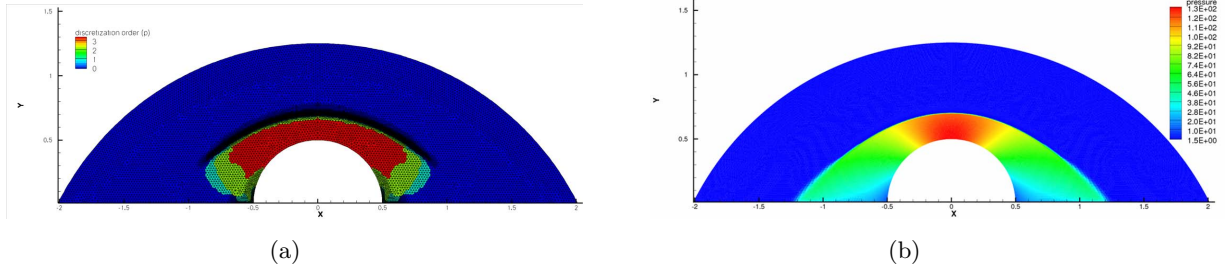
### 3.2 High Speed Flows

One of the principal objectives of this work was to quantify errors in the simulation of hypersonic flows and to use this information to reduce simulation uncertainty. Two different tasks were carried out: the first concentrated on the effects of spatial discretization error using a perfect gas model for simplicity, and the second concentrated on errors due to parameter uncertainties in real gas models while ignoring discretization errors.

#### 3.2.1 Spatial Discretization Error Control

The spatial discretization error work relied on a high-order accurate discontinuous Galerkin (DG) discretization scheme using the Euler equations in two dimensions. The considered objective was the surface integrated temperature on a cylinder subjected to a hypersonic flow (Mach 6 or Mach 10) using the perfect gas assumption. The error in the surface temperature objective due to discretization error in the mesh was estimated by computing the adjoint of this objective and forming the inner product of this adjoint field with the non-zero residual of the current solution projected onto a finer grid. The distribution of this error in space provides a criterion for adaptively refining the mesh (h-refinement) or locally raising the order of approximation (p-refinement). The choice between h and p refinement is determined by examining the local smoothness of the solution, as determined either by the decay of the higher-order modal coefficients, or by the magnitude of the jumps between neighboring mesh elements.

The procedure starts with a first-order accurate discretization on a coarse mesh, and proceeds to raise the order or refine the mesh in regions of large spatial error. Because shock wave regions are always flagged as non-smooth regions, the solution naturally remains first-order accurate in these regions, increased accuracy is obtained through h refinement in these regions, and solution limiting procedures are not required. This approach has been applied to Mach 6 flow over a cylinder, using the surface integrated temperature as the functional output of interest for the refinement process, and Mach 10 flow, using the cylinder drag as the functional output of interest. Figure 2 illustrates the mesh, accuracy order and final solution for this case, showing extensive mesh refinement in the shock region, and high-order accuracy ahead of the cylinder. Note that no h or p refinement occurs at lateral locations near the cylinder, since the flow in these areas does not impinge upon the cylinder, and therefore does not affect the functional of interest. The resulting procedure is capable of capturing the shock with no limiting while providing high accuracy due to the selective application of h and p refinement. On the other hand, robustness issues have been encountered in situations where the shock moves into a higher-order p region due to convergence transients. Therefore, it is anticipated that a combination of the filtering and/or artificial dissipation techniques discussed above may be required to enhance the robustness of this approach. Results from this work are summarized in a references [2,10].



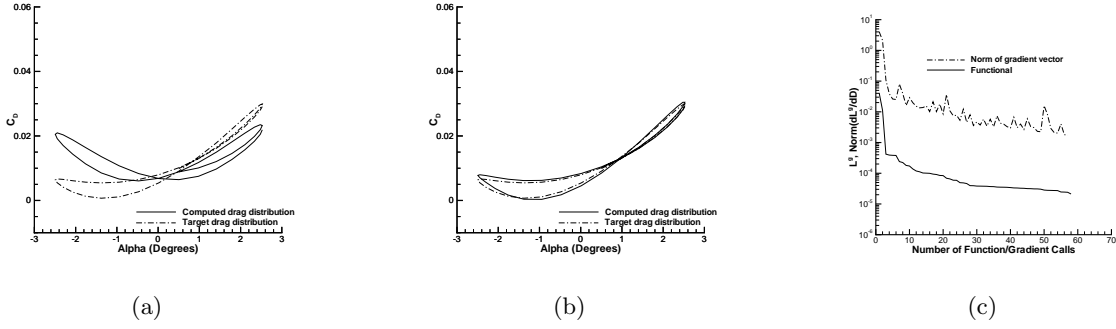
**Figure 2:** (a) Resulting mesh and order of accuracy for adaptive h-p simulation of Mach 10 flow over cylinder; (b) Computed flow field for h-p adaptive simulation of Mach 10 flow over cylinder

### 3.2.2 Uncertainty due to Real Gas Model Parameters

A large source of uncertainty for realistic hypersonic simulations rests with the use of empirically determined real gas model parameters such as reaction rates and transport coefficients. This has been mentioned in a survey paper co-authored by the PI and G. Candler [8]. Because real gas models contain a large number of model parameters, adjoint methods provide an efficient strategy for determining the effect of all model parameter uncertainties on important simulation objectives such as surface heating. Solution of the adjoint problem provides the first derivative of the targeted objective with respect to all model parameters at the cost of a single adjoint problem, which is roughly equivalent to the cost of the original flow analysis. Once these first-order sensitivities are known, they can be used to identify the most important model parameters for further study, or they can be used to perform uncertainty quantification through gradient enhanced inexpensive Monte-Carlo methods, or gradient enhanced non-intrusive polynomial chaos methods. However, to be effective, adjoint methods must be closely coupled with the original simulation code, i.e. they require the linearization of the analysis code. In order to study the feasibility of obtaining sensitivities of heating objectives with respect to real gas model parameters, an in-house two-dimensional real gas Navier-Stokes hypersonic solver was constructed from scratch along with the adjoint of each important functional module of this simulation code, thus providing an efficient adjoint capability for real gas problems. This code was first validated in analysis mode against well known simulation results from LAURA and FUN2D, and then used to compute the hypersonic flow over a two-dimensional cylinder and the adjoint of the surface integrated heating objective, which was then used to produce the first-order sensitivities of the heating objective with respect to 34 different chemical reaction rate parameters, and 15 different model parameters required in the definition of the transport coefficients in the real gas model. The findings indicated that the reaction rates governing the formation and breakdown of nitrous-oxide and the recombination of oxygen were the most sensitive with regards to surface heating. This work was documented in reference [6] and is being extended to enable enhanced uncertainty quantification methods using the sensitivity information derived through the adjoint approach described herein.

### 3.3 Unsteady Flows

Another major focus of this project was the development and demonstration of adjoint techniques for unsteady problems and multidisciplinary problems. For unsteady problems, the adjoint formulation results in a recurrence relation in time which must be solved through backsubstitution, which is analogous to a backwards integration in time of the adjoint equations. For multidisciplinary prob-



**Figure 3:** Illustration of time-dependent optimization problem for two-dimensional pitching airfoil. (a) Initial computed time-dependent drag profile and target profile; (b) Computed drag profile and target drag profile after 58 design cycles; (c) Convergence of optimization procedure as measured by decrease of objective functional using LBFGS optimization package.

lems, each disciplinary adjoint must be formulated and the fully coupled adjoint system involving all disciplines must be solved in a manner analogous to the solution of the fully coupled multidisciplinary analysis problem. During the first part of this project, we have developed a modular framework for deriving and solving the adjoint problem for complex simulation problems which may involve unsteady and multidisciplinary components. This formulation was then used to implement and solve the adjoint problem for unsteady flows, firstly in two dimensions [1,4,13], secondly in three dimensions [12], and then was extended (in two dimensions) to the multidisciplinary problem of aeroelasticity where the fully coupled structural and fluid flow unsteady adjoint have been solved [3,11].

The unsteady adjoint was initially used to demonstrate the solution of time-dependent optimization problems for a pitching airfoil problem [4]. A time-integrated objective was formulated as the RMS difference over the time domain between the computed lift and drag profiles of the initial airfoil and specified target lift and drag profiles. The airfoil shape is then modified in order to minimize this objective using a gradient-based optimization procedure relying on the gradients computed via the unsteady adjoint formulation. This process is illustrated in Figure 3. The initial airfoil consists of a NACA 0012 airfoil in a Mach 0.755 flow, pitching about a mean angle of incidence of  $0.016^\circ$  with  $2.51^\circ$  amplitude, at a reduced frequency of 0.0814. The initial computed time-dependent drag profile for this case is shown in Figure 3(a), along with the target drag distribution. Both target lift and drag distributions are specified in the objective, although only the drag profiles are shown here for brevity. After 58 design cycles, the airfoil shape has been modified such that the computed drag profile agrees much more closely with the target drag profile as shown in Figure 3(b). Figure 3(c) depicts the convergence of the optimization process, where the objective is seen to be reduced by four orders of magnitude over 58 design cycles using the LBFGS optimization package. In general, unsteady optimization problems have been found to be substantially more difficult to solve than steady-state optimization problems, requiring relatively sophisticated optimizers such as LBFGS, and large numbers of design cycles (58 in this case). Attempts to drive this optimization problem with simple methods such as steepest-descent have proved to be relatively ineffective. The same modular adjoint formulation has also been extended to multidisciplinary aeroelasticity problems,



where the adjoint of the full coupled aerodynamic and structural problem has been derived, and used to perform shape optimization for flutter suppression [3,11].

Another application of the time-dependent adjoint can be found in its use for temporal error estimation. In references [1,13] we have shown how the unsteady adjoint can be used to estimate global temporal error in a target simulation objective for various aerodynamic problems including the interaction of a vortex and a two-dimensional airfoil, and used to adaptively refine the time-step distribution to reduce the overall objective error. Furthermore, it was shown how the adjoint can also be used to estimate algebraic error in the simulation objective due to incomplete convergence of the implicit system at each time step, and thus guide convergence tolerance decisions, an important practical problem which has received relatively little attention in the past. The results from these investigations have shown that multiple error sources can be estimated accurately and controlled robustly with this approach.

#### 4. People Supported

This project supported one postdoctoral researcher Zhi Yang on a part-time basis. Zhi Yang has been instrumental in developing the adjoint optimized mesh motion technique in the first year of this project [5,14]. He has also assisted with the graduate students supported by this project. PhD student Karthik Mani was supported under this project and completed his PhD thesis during that time. He developed most of the techniques for formulating and solving the unsteady adjoint equations and applying these to optimization, error control, and aeroelasticity problems [1,3,4,7,9,11,13]. PhD student Li Wang was partly supported on this project and demonstrated the use of h-p adaptivity driven by the adjoint for hypersonic problems [2,10]. PhD Brian Lockwood was not directly supported by this project but contributed technically through his development of an in-house real gas hypersonic code (two-dimensional) and the formulation and solution of the real gas sensitivities using the adjoint approach [6]. Finally, the PI (Mavriplis) was supported during one summer month each year. He spend considerable time working with the postdoc and students, but also contributed directly through his implementation of the unsteady adjoint method into the three dimensional unstructured Navier-Stokes code NSU3D [12].

#### 5. Interactions

Throughout the course of this project, our research results were disseminated through attendance and presentations at conferences, other invited presentations, and publication of our papers. Presentations were delivered at the 2007, 2008, 2009 and 2010 AIAA Aerospace Sciences meetings, as well as at the 2007 AIAA Computational Fluid Dynamics Meeting, and the 2008 Applied Aerodynamics Meeting. Interactions with AFRL at WPAFB were on-going, with several visits by the PI (Mavriplis) during the project. In May 2009, Mavriplis gave an invited lecture at the Workshop on Uncertainty Quantification Methods held in Dayton OH, and returned to AFRL in June 2009 to give a briefing on sensitivity analysis methods using adjoint techniques to the staff in the Air Vehicles Directorate at AFRL at WPAFB. Yearly summer visits to NASA Langley were also undertaken by the PI and in 2009 two PhD students were invited to spend two weeks at NASA Langley and present their work on hypersonic adjoint simulations and progress in discontinuous Galerkin methods. PI Mavriplis attended the AFOSR contractor meeting each year of the project which was co-located with the NASA hypersonics program review in the last two years, which also funds a portion of the PIs research program. Li Wang obtained her PhD in May 2009 and was hired as a research professor in the Simulation Center at the University of Tennessee at Chattanooga,

and continues her research in this area. Karthik Mani, who also obtained his PhD in May 2009 was hired into the PI's research group as a postdoctoral researcher and is currently extending his research results developed under this project into three dimensions for use in practical applications.

## **6. Publications**

This project has resulted in the publication of 5 archival journal articles, in AIAA Journal and the Journal of Computational Physics. A total of 9 conference publications, principally AIAA conference papers have been presented and published. Finally, two student PhD theses were produced during this project. A list of all publications produced during this project is given below.

### Journal Publications:

1. Mani, K. and Mavriplis, D. J., "Error Estimation and Adaptation for Functional Output in Time-Dependent Flow Problems", *Journal of Computational Physics*, Vol 229, No. 2, pp. 415-440, January 2010.
2. Wang, L. and Mavriplis, D. J., "Adjoint-Based h-p Adaptive Discontinuous Galerkin Methods for the 2D Compressible Euler Equations", *Journal of Computational Physics*, Vol 228, No. 20, pp. 7643-7661, November 2009.
3. Mani, K. and Mavriplis, D. J., "Adjoint-Based Sensitivity Formulation for Fully Coupled Unsteady Aeroelasticity Problems", *AIAA Journal*, Vol. 47, No. 8, pp. 1902-1915, August 2009.
4. Mani, K. and Mavriplis, D. J., "Unsteady Discrete Adjoint Formulation for Two- Dimensional Flow Problems with Deforming Meshes", *AIAA Journal*, Vol 46, No. 6, pp. 1351 - 1364, June 2008.
5. Yang, Z. and Mavriplis, D. J., "A Mesh Deformation Strategy Optimized by the Adjoint Method on Unstructured Meshes", *AIAA Journal*, Vol 45, No. 12, pp. 2885 - 2896, December 2007.

### Conference Papers:

6. Lockwood, B., and Mavriplis, D. J., "Parameter Sensitivity Analysis for Hypersonic Viscous Flow using a Discrete Adjoint Approach", *AIAA Paper 2010-447*, Presented at the 48th AIAA Aerospace Sciences Meeting, Orlando FL, January 2010.
7. Mani, K. and Mavriplis, D. J., "Spatially Non-Uniform Time-Step Adaptation for in Unsteady Flow Problems", Paper delivered at the 21st Century Challenges in Computational Engineering and Science, Workshop held at Princeton University, November 2009.
8. Candler, G., Mavriplis, D. J., and Trevino, L., "Current Status and Future Prospects for the Numerical Simulation of Hypersonic Flows", *AIAA Paper 2009-0153*, presented at the 47<sup>th</sup> AIAA Aerospace Sciences Meeting, Orlando FL, January, 2009.
9. Mani, K. and Mavriplis, D. J., "Error Estimation and Adaptation for Functional Outputs in Time Dependent Flow Problems", *AIAA Paper 2009-1495*, presented at the 47<sup>th</sup> AIAA Aerospace Sciences Meeting, Orlando FL, January, 2009.
10. Wang, L., and Mavriplis, D. J., "Adjoint-Based h-p Adaptive Discontinuous Galerkin Methods for Aerospace Applications", *AIAA 2009-0952*, presented at the 47<sup>th</sup> AIAA Aerospace Sciences Meeting, Orlando FL, January, 2009.
11. Mani, K. and Mavriplis, D. J., "Linearization of the Coupled Unsteady Fluid-Structure Equations: Application to Flutter Control", *AIAA paper 2008-6242*, 26th AIAA Applied Aerodynamics Conference, Honolulu, Hawaii, Aug. 18-21, 2008.
12. Mavriplis, D. J., "Solution of the Unsteady Discrete Adjoint for Three-Dimensional Problems on Dynamically Deforming Unstructured Meshes", *AIAA paper 2008-727*, 46th AIAA Aerospace Sciences Meeting and Exhibit, Reno, Nevada, Jan. 7-10, 2008.
13. Mani, K., and Mavriplis, D. J. "Discrete Adjoint-Based Time-Step Adaptation and Error Reduction in Unsteady Flow Problems", *AIAA Paper 2007-3944*, paper presented at the 18th AIAA CFD Conference, Miami, FL, June 2007.
14. Yang, Z. and Mavriplis, D. J., "A Mesh Deformation Strategy Optimized by the Adjoint Method on Unstructured Meshes ", *AIAA Paper 2007-0557*, presented at the 45<sup>th</sup> AIAA Aerospace Sciences Meeting, Reno NV, January 2007.

**Student Theses:**

**Karthik Mani:**

Admission: September 2005

Graduation: May 2009

Thesis:

*Application of the Discrete Adjoint Method to Coupled Multidisciplinary Unsteady Flow Problems for Error Estimation and Optimization* Karthik Mani, PhD Thesis, Department of Mechanical Engineering, University of Wyoming, May 2009. 220 pages

**Li Wang:**

Admission: January 2004

Graduation: PhD May 2009

Thesis:

*Techniques for High-Order Adaptive Discontinuous Galerkin Discretizations in Fluid Dynamics.* Li Wang, PhD Thesis, Department of Mechanical Engineering, University of Wyoming, May 2009. 190 pages.